

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 07:19:28 ON 07 MAY 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.42

0.42

FILE 'REGISTRY' ENTERED AT 07:20:51 ON 07 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

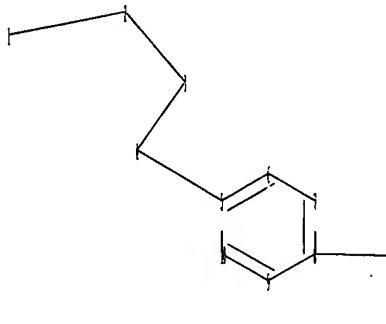
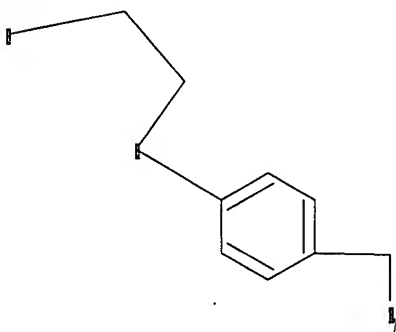
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 2.str



chain nodes :

1 2 3 4 11 12

ring nodes :

5 6 7 8 9 10

chain bonds :  
 1-2 2-3 3-4 4-5 8-11 11-12  
 ring bonds :  
 5-6 5-10 6-7 7-8 8-9 9-10  
 exact/norm bonds :  
 1-2 3-4 4-5 11-12  
 exact bonds :  
 2-3 8-11  
 normalized bonds :  
 5-6 5-10 6-7 7-8 8-9 9-10

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 07:21:27 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 3363 TO ITERATE

59.5% PROCESSED 2000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

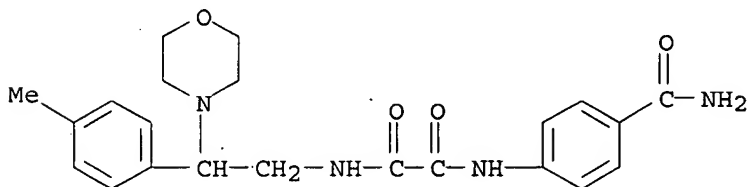
39 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 63782 TO 70738  
 PROJECTED ANSWERS: 826 TO 1796

L2 39 SEA SSS SAM L1

=> d 1-39

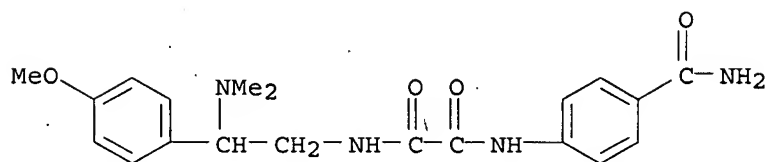
L2 ANSWER 1 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 920259-55-8 REGISTRY  
 ED Entered STN: 09 Feb 2007  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C22 H26 N4 O4  
 SR Chemical Library  
 Supplier: Aurora Fine Chemicals



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

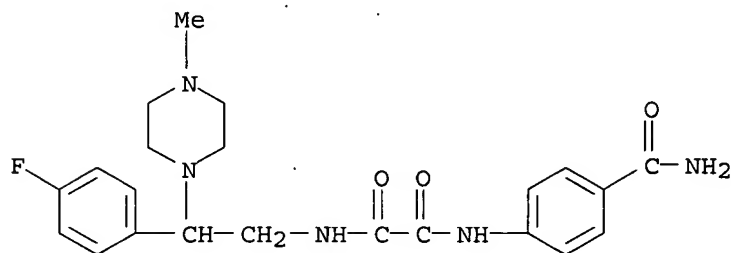
L2 ANSWER 2 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 920258-02-2 REGISTRY  
 ED Entered STN: 09 Feb 2007  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C20 H24 N4 O4

SR Chemical Library  
Supplier: Aurora Fine Chemicals



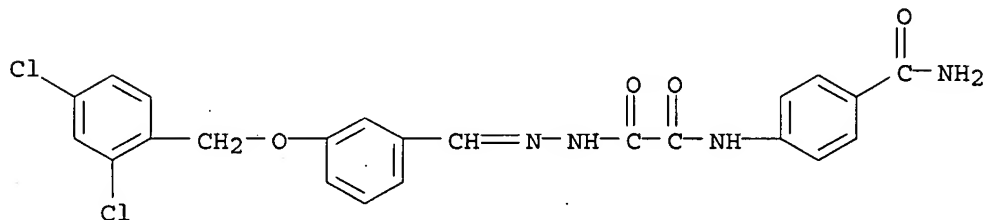
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 3 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 906151-24-4 REGISTRY  
ED Entered STN: 10 Sep 2006  
CN INDEX NAME NOT YET ASSIGNED  
MF C22 H26 F N5 O3  
SR Chemical Library  
Supplier: Ambinter



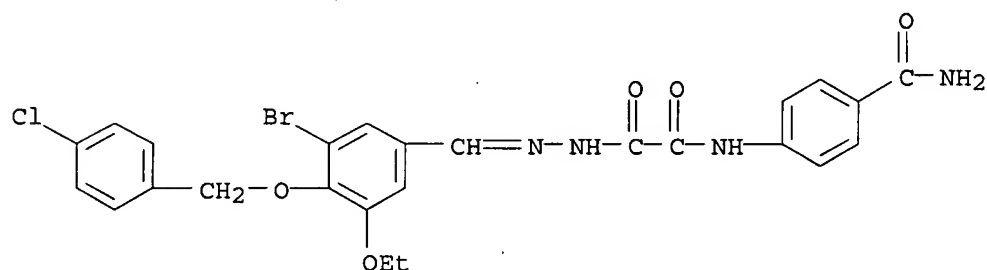
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 4 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 885559-11-5 REGISTRY  
ED Entered STN: 25 May 2006  
CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-[(2,4-dichlorophenyl)methoxy]phenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
MF C23 H18 Cl2 N4 O4  
SR Chemical Library  
Supplier: Scientific Exchange, Inc.  
LC STN Files: CHEMCATS



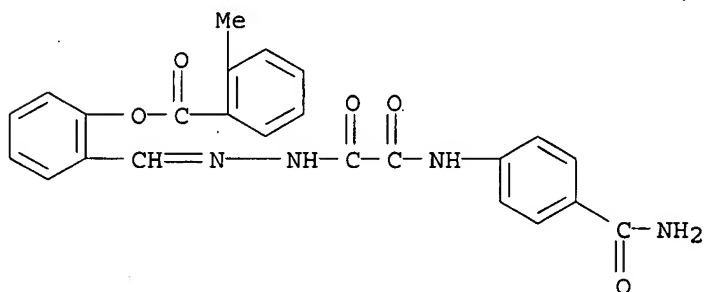
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 5 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885551-73-5 REGISTRY  
 ED Entered STN: 25 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-bromo-4-[(4-chlorophenyl)methoxy]-5-ethoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
 MF C25 H22 Br Cl N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



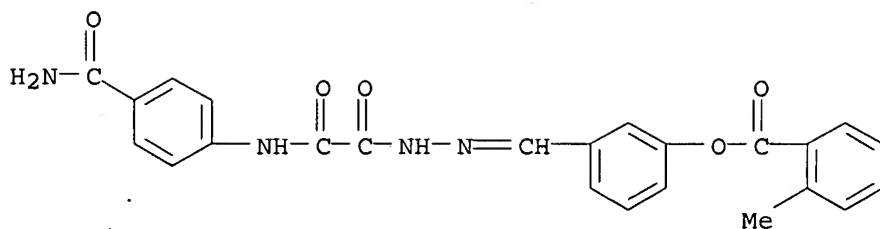
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 6 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885546-88-3 REGISTRY  
 ED Entered STN: 25 May 2006  
 CN Benzoic acid, 2-methyl-, 2-[[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazono]methyl]phenyl ester (9CI) (CA INDEX NAME)  
 MF C24 H20 N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



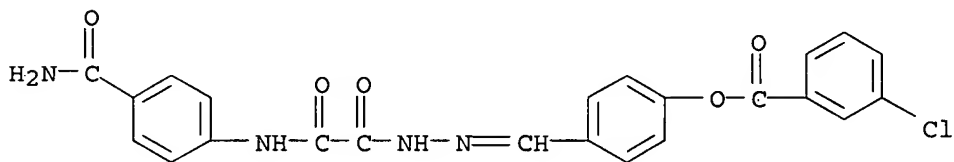
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 7 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885534-75-8 REGISTRY  
 ED Entered STN: 25 May 2006  
 CN Benzoic acid, 2-methyl-, 3-[[[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazono]methyl]phenyl ester (9CI) (CA INDEX NAME)  
 MF C24 H20 N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



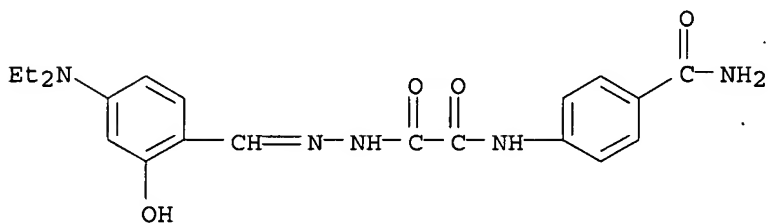
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 8 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885188-00-1 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Benzoic acid, 3-chloro-, 4-[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazone]methyl]phenyl ester (9CI) (CA INDEX NAME)  
 MF C23 H17 Cl N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

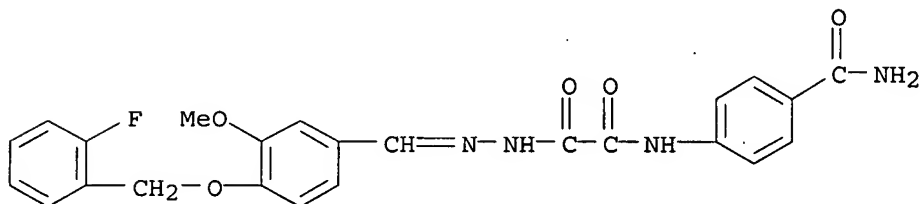
L2 ANSWER 9 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885184-92-9 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-(diethylamino)-2-hydroxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
 MF C20 H23 N5 O4  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

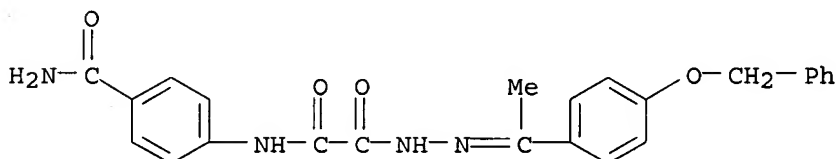
L2 ANSWER 10 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885183-17-5 REGISTRY

ED Entered STN: 22 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-[(2-fluorophenyl)methoxy]-3-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
 MF C24 H21 F N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



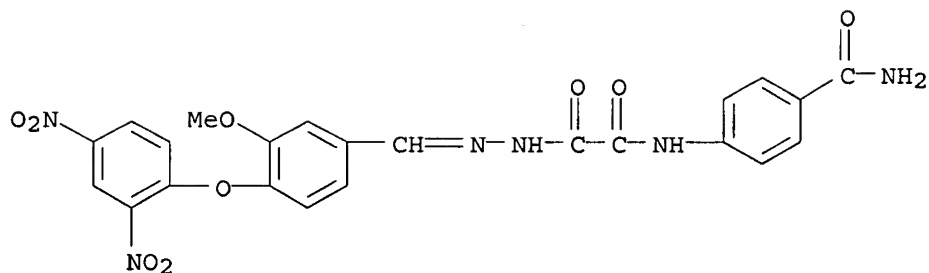
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 11 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885167-04-4 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [1-[4-(phenylmethoxy)phenyl]ethylidene]hydrazide (9CI) (CA INDEX NAME)  
 MF C24 H22 N4 O4  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



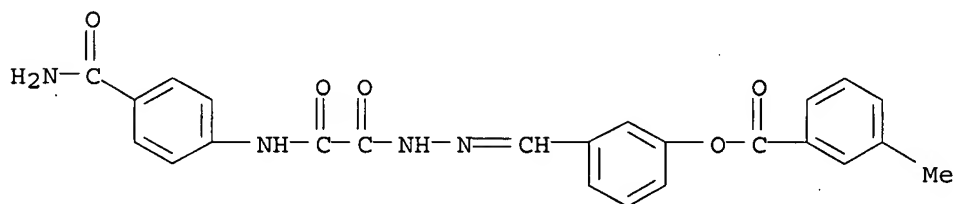
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 12 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885162-48-1 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[4-(2,4-dinitrophenoxy)-3-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
 MF C23 H18 N6 O9  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



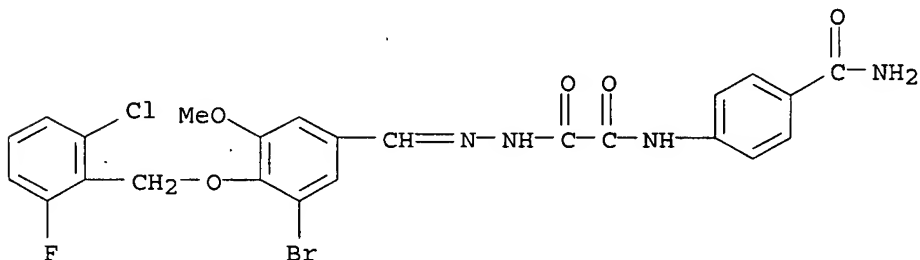
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 13 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885161-26-2 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Benzoic acid, 3-methyl-, 3-[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazono]methyl]phenyl ester (9CI) (CA INDEX NAME)  
 MF C24 H20 N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



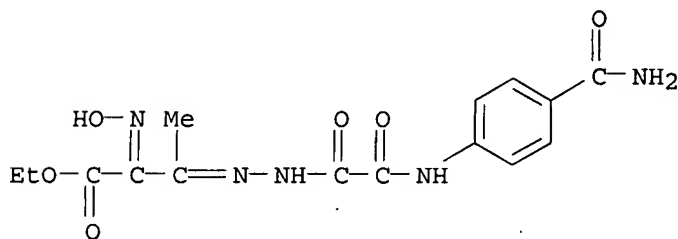
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 14 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885154-04-1 REGISTRY  
 ED Entered STN: 22 May 2006  
 CN Acetic acid, [[4-(aminocarbonyl)phenyl]amino]oxo-, [[3-bromo-4-[(2-chloro-6-fluorophenyl)methoxy]-5-methoxyphenyl]methylene]hydrazide (9CI) (CA INDEX NAME)  
 MF C24 H19 Br Cl F N4 O5  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



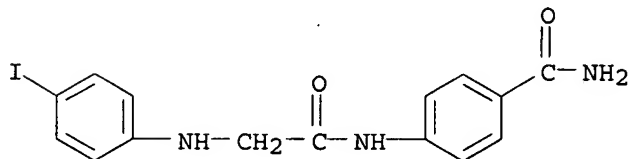
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 15 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 885139-62-8 REGISTRY  
ED Entered STN: 22 May 2006  
CN Butanoic acid, 3-[[[4-(aminocarbonyl)phenyl]amino]oxoacetyl]hydrazono]-2-(hydroxyimino)-, ethyl ester (9CI) (CA INDEX NAME)  
MF C15 H17 N5 O6  
SR Chemical Library  
Supplier: Scientific Exchange, Inc.  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

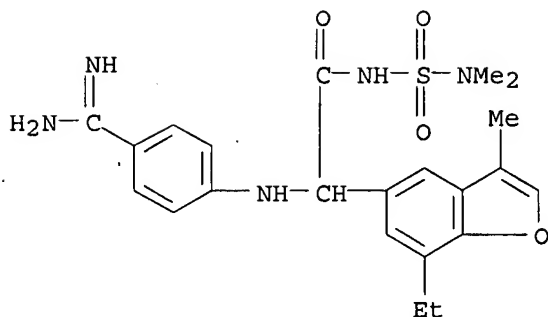
L2 ANSWER 16 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 850215-90-6 REGISTRY  
ED Entered STN: 11 May 2005  
CN Benzamide, 4-[[[(4-iodophenyl)amino]acetyl]amino]- (9CI) (CA INDEX NAME)  
MF C15 H14 I N3 O2  
SR Chemical Library  
Supplier: Enamine



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 17 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 797784-55-5 REGISTRY  
ED Entered STN: 15 Dec 2004  
CN 5-Benzofuranacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-N-[(dimethylamino)sulfonyl]-7-ethyl-3-methyl- (9CI) (CA INDEX NAME)  
MF C22 H27 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



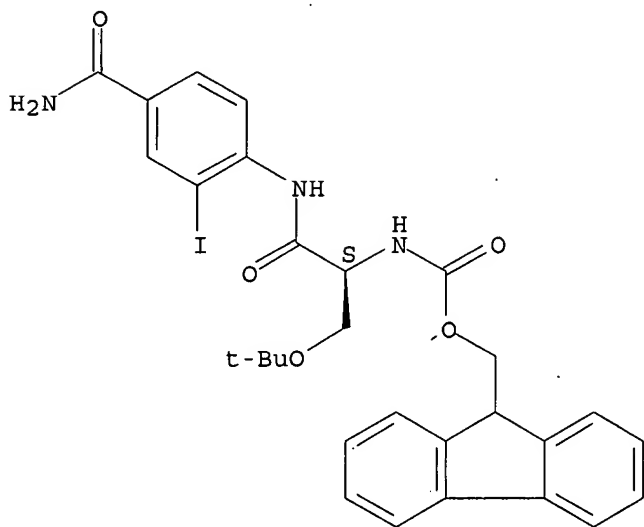


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 18 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 503130-93-6 REGISTRY  
ED Entered STN: 16 Apr 2003  
CN Carbamic acid, [(1S)-2-[[4-(aminocarbonyl)-2-iodophenyl]amino]-1-[(1,1-dimethylethoxy)methyl]-2-oxoethyl]-, 9H-fluoren-9-ylmethyl ester (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C29 H30 I N3 O5  
SR CA  
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

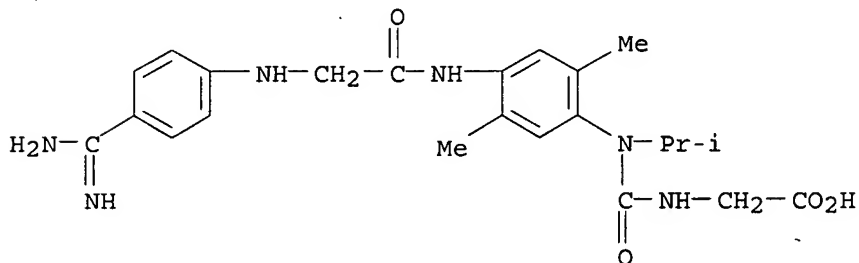


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 19 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 481069-24-3 REGISTRY

ED Entered STN: 24 Jan 2003  
 CN Glycine, N-[[[4-[[[4-(aminoiminomethyl)phenyl]amino]acetyl]amino]-2,5-dimethylphenyl](1-methylethyl)amino]carbonyl]- (9CI) (CA INDEX NAME)  
 MF C23 H30 N6 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

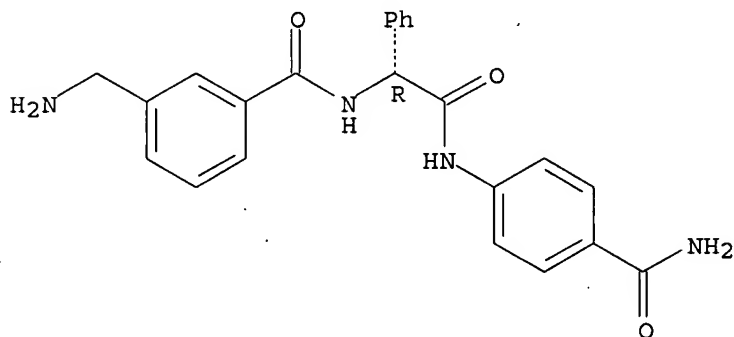
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 20 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 313491-49-5 REGISTRY  
 ED Entered STN: 11 Jan 2001  
 CN Benzeneacetamide, N-[4-(aminocarbonyl)phenyl]-α-[[3-(aminomethyl)benzoyl]amino]-, (αR)-, mono(trifluoroacetate) (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C23 H22 N4 O3 . C2 H F3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS

CM 1

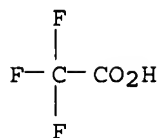
CRN 313491-48-4  
 CMF C23 H22 N4 O3

Absolute stereochemistry.



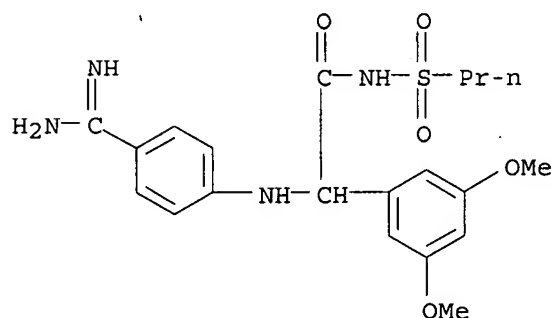
CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



3 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

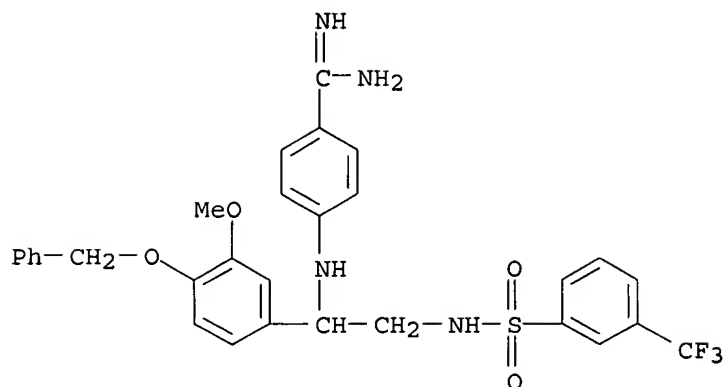
L2 ANSWER 21 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 284044-11-7 REGISTRY  
ED Entered STN: 08 Aug 2000  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-3,5-dimethoxy-N-(propylsulfonyl)- (9CI) (CA INDEX NAME)  
MF C20 H26 N4 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

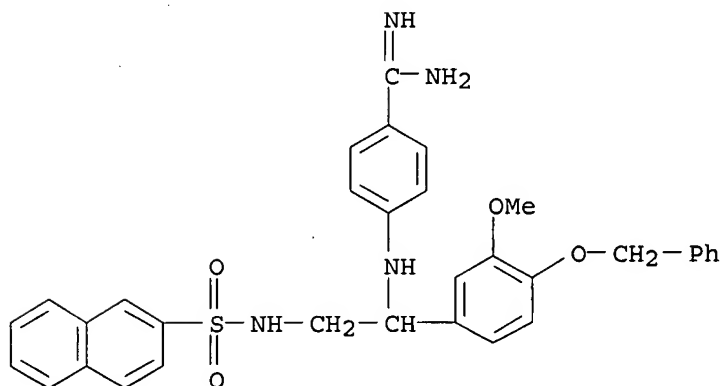
L2 ANSWER 22 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 284043-72-7 REGISTRY  
ED Entered STN: 08 Aug 2000  
CN Benzenecarboximidamide, 4-[[1-[3-methoxy-4-(phenylmethoxy)phenyl]-2-[[[3-(trifluoromethyl)phenyl]sulfonyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)  
MF C30 H29 F3 N4 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

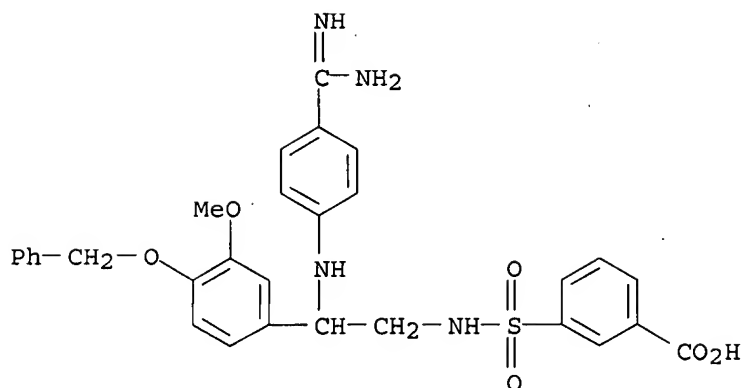
L2 ANSWER 23 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 284043-68-1 REGISTRY  
ED Entered STN: 08 Aug 2000  
CN Benzenecarboximidamide, 4-[[1-[[3-methoxy-4-(phenylmethoxy)phenyl]amino]ethyl]amino]-2-[(2-naphthalenylsulfonyl)amino]ethyl]amino]- (9CI) (CA INDEX NAME)  
MF C33 H32 N4 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

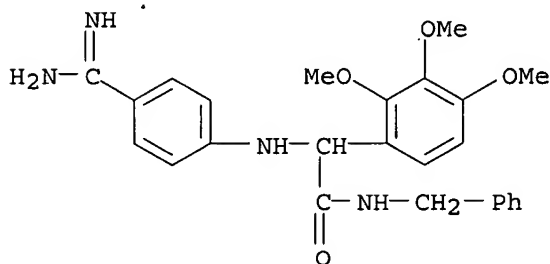
L2 ANSWER 24 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 284043-62-5 REGISTRY  
ED Entered STN: 08 Aug 2000  
CN Benzoic acid, 3-[[[2-[[4-(aminoiminomethyl)phenyl]amino]-2-[3-methoxy-4-(phenylmethoxy)phenyl]ethyl]amino]sulfonyl]- (9CI) (CA INDEX NAME)  
MF C30 H30 N4 O6 S  
SR CA  
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

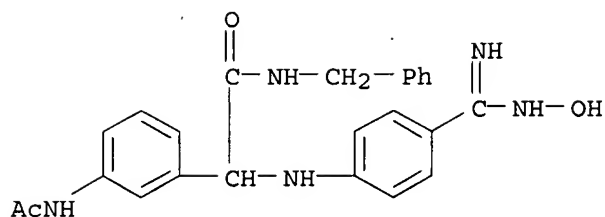
L2 ANSWER 25 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227024-17-1 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-2,3,4-trimethoxy-N-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)  
MF C25 H28 N4 O4 . x Cl H  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
CRN (709608-58-2)



● x HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 26 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227023-65-6 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide, 3-(acetylamino)- $\alpha$ -[[4-[(hydroxyamino)iminomethyl]phenyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)  
MF C24 H25 N5 O3  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

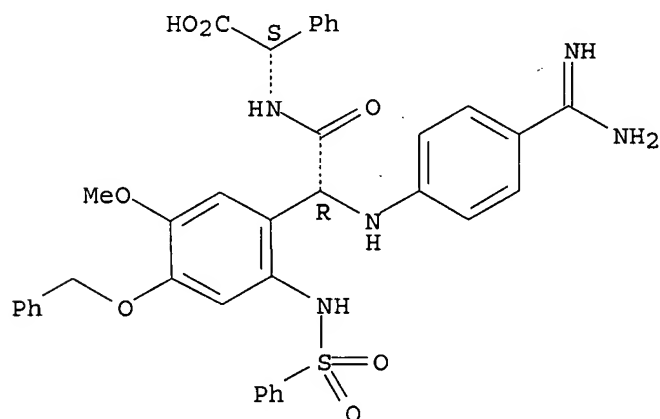


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 27 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227023-17-8 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Glycine, (2R)-N-[4-(aminoiminomethyl)phenyl]-2-[5-methoxy-4-(phenylmethoxy)-2-[(phenylsulfonyl)amino]phenyl]glycyl-2-phenyl-, (2S)-(9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C37 H35 N5 O7 S  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

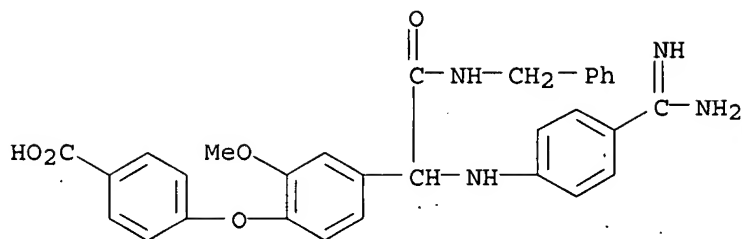
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

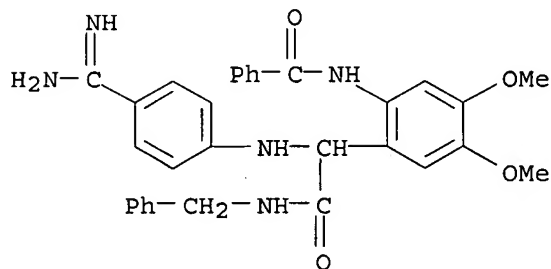
L2 ANSWER 28 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227023-06-5 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzoic acid, 4-[4-[1-[[4-(aminoiminomethyl)phenyl]amino]-2-oxo-2-[(phenylmethyl)amino]ethyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)  
MF C30 H28 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 29 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227022-78-8 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-2-(benzoylamino)-4,5-dimethoxy-N-(phenylmethyl)- (9CI) (CA INDEX NAME)  
MF C31 H31 N5 O4  
CI COM  
SR CA



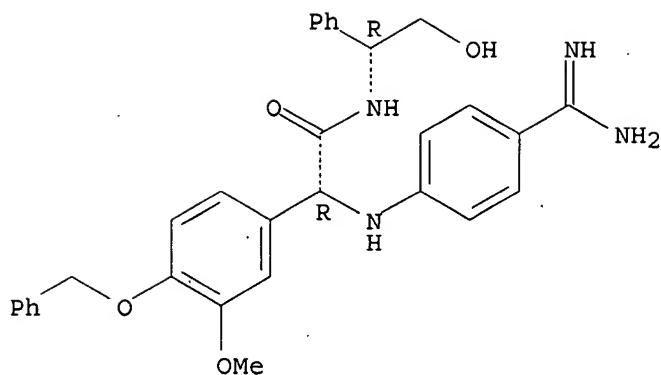
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 30 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227022-63-1 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-N-[(1R)-2-hydroxy-1-phenylethyl]-3-methoxy-4-(phenylmethoxy)-, ( $\alpha$ R)-, monoacetate (salt) (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H32 N4 O4 . C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 227022-62-0  
CMF C31 H32 N4 O4

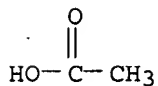
Absolute stereochemistry.



CM 2

CRN 64-19-7

CMF C2 H4 O2



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 31 OF 39. REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-41-5 REGISTRY

ED Entered STN: 07 Jul 1999

CN Butanoic acid, 4-amino-2-[[[4-(aminoiminomethyl)phenyl]amino][3-methoxy-4-(phenylmethoxy)phenyl]acetyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

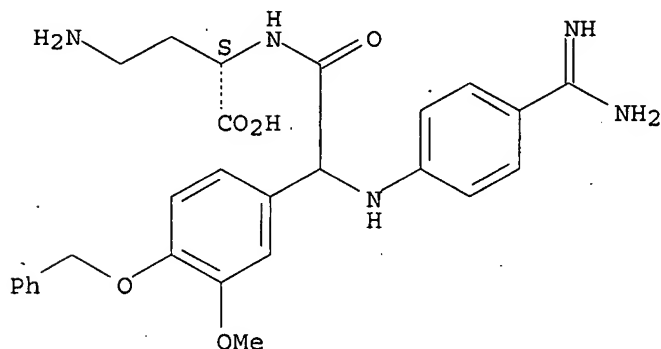
FS STEREOSEARCH

MF C27 H31 N5 O5

CI COM

SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 32 OF 39. REGISTRY COPYRIGHT 2007 ACS on STN

RN 227022-29-9 REGISTRY

ED Entered STN: 07 Jul 1999

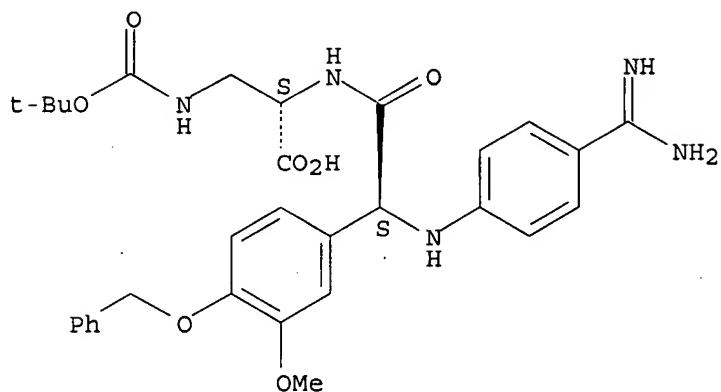
CN L-Alanine, (2S)-N-[4-(aminoiminomethyl)phenyl]-2-[3-methoxy-4-



(phenylmethoxy)phenyl]glycyl-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH  
MF C31 H37 N5 O7  
CI COM  
SR CA

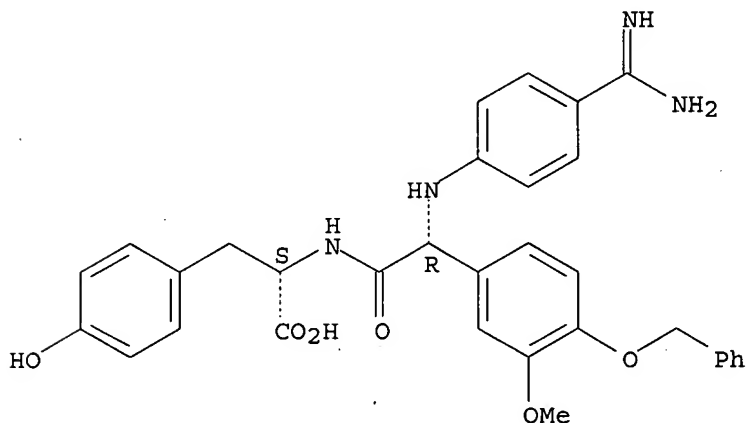
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 33 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227021-99-0 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN L-Tyrosine, (2R)-N-[4-(aminoiminomethyl)phenyl]-2-[3-methoxy-4-(phenylmethoxy)phenyl]glycyl- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C32 H32 N4 O6  
CI COM  
SR CA

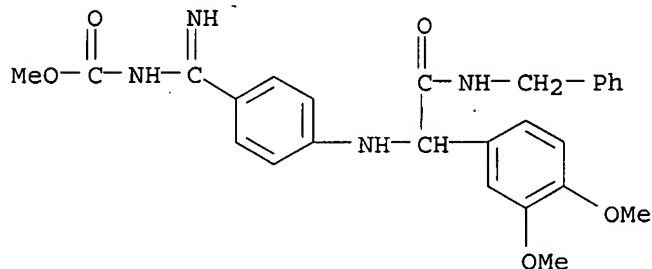
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 34 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227021-88-7 REGISTRY  
ED Entered STN: 07 Jul 1999

CN Carbamic acid, [[4-[[1-(3,4-dimethoxyphenyl)-2-oxo-2-  
 [(phenylmethyl)amino]ethyl]amino]phenyl]iminomethyl]-, methyl ester (9CI)  
 (CA INDEX NAME)  
 MF C26 H28 N4 O5  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



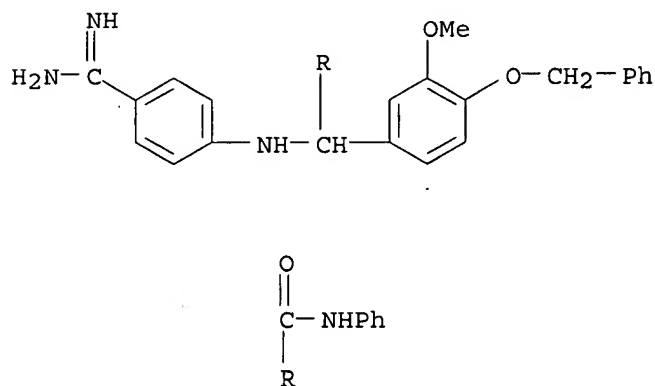
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 35 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 227021-10-5 REGISTRY  
 ED Entered STN: 07 Jul 1999  
 CN Benzeneacetamide, α-[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-N-  
 phenyl-4-(phenylmethoxy)-, acetate (9CI) (CA INDEX NAME)  
 MF C29 H28 N4 O3 . x C2 H4 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

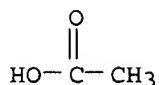
CM 1

CRN 227021-09-2  
 CMF C29 H28 N4 O3



CM 2

CRN 64-19-7  
 CMF C2 H4 O2

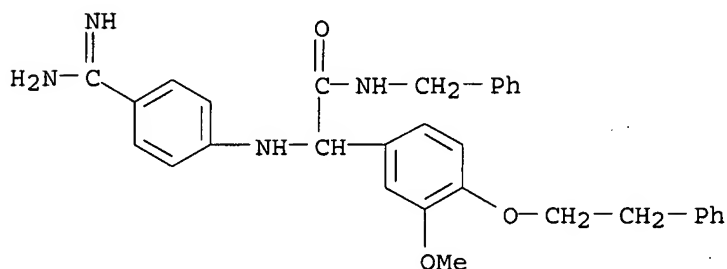


1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 36 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227020-88-4 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-(2-phenylethoxy)-N-(phenylmethyl)-, acetate (9CI) (CA INDEX NAME)  
MF C31 H32 N4 O3 . x C2 H4 O2  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

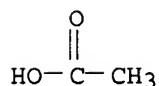
CM 1

CRN 227020-87-3  
CMF C31. H32 N4 O3



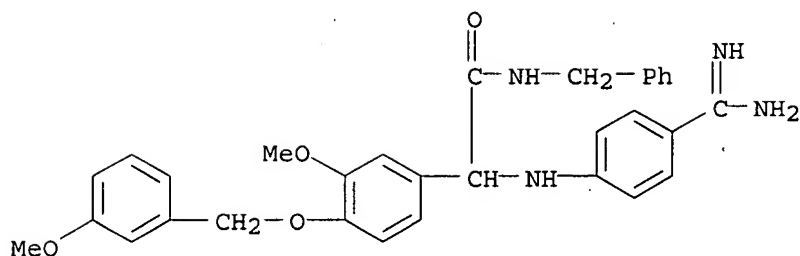
CM 2

CRN 64-19-7  
CMF C2 H4 O2



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 37 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 227020-71-5 REGISTRY  
ED Entered STN: 07 Jul 1999  
CN Benzeneacetamide,  $\alpha$ -[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-[(3-methoxyphenyl)methoxy]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)  
MF C31 H32 N4 O4  
CI COM  
SR CA

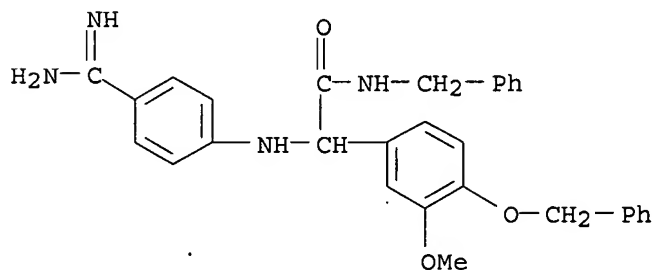


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 38 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 227020-58-8 REGISTRY  
 ED Entered STN: 07 Jul 1999  
 CN Benzeneacetamide, α-[[4-(aminoiminomethyl)phenyl]amino]-3-methoxy-4-(phenylmethoxy)-N-(phenylmethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)  
 MF C30 H30 N4 O3 . x C2 H F3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL

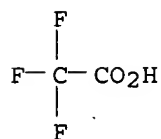
CM 1

CRN 227020-57-7  
 CMF C30 H30 N4 O3



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 39 OF 39 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 90291-90-0 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN Benzenepropanamide, N-[4-(aminoiminomethyl)phenyl]-α-[[4-(methylphenyl)sulfonyl]amino]-, monohydriodide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

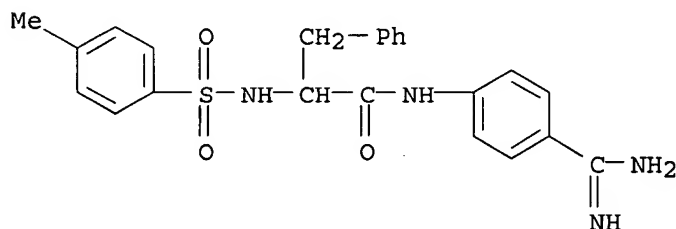
CN Benzenepropanamide, N-[4-(aminoiminomethyl)phenyl]- $\alpha$ -[[4-methylphenyl)sulfonyl]amino]-, monohydriodide, ( $\pm$ )-

MF C23 H24 N4 O3 S . H I

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

CRN (92953-67-8)



● HI

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s 11 esa

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> s 11 exa

SAMPLE SEARCH INITIATED 07:23:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

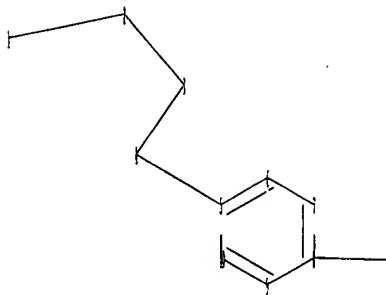
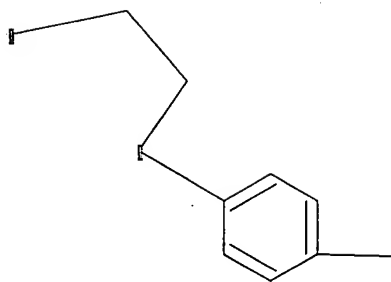
PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L3 0 SEA EXA SAM L1

=>

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 3.str



```

chain nodes :
1  2  3  4 11
ring nodes :
5  6  7  8  9 10
chain bonds :
1-2  2-3  3-4  4-5  8-11
ring bonds :
5-6  5-10  6-7  7-8  8-9  9-10
exact/norm bonds :
1-2  3-4  4-5
exact bonds :
2-3  8-11
normalized bonds :
5-6  5-10  6-7  7-8  8-9  9-10

```

Match level :

```

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS

```

L4 STRUCTURE UPLOADED

```

=> s l4 exa
SAMPLE SEARCH INITIATED 07:24:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

```

```

100.0% PROCESSED          5 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

```

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   5 TO      234
PROJECTED ANSWERS:      0 TO      0

```

L5 0 SEA EXA SAM L4

```

=> s l4 full
FULL SEARCH INITIATED 07:24:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 126827 TO ITERATE

```

```

100.0% PROCESSED 126827 ITERATIONS 25959 ANSWERS
SEARCH TIME: 00.00.02

```

L6 25959 SEA SSS FUL L4

```

=> s l6 esa
MISSING OPERATOR

```

```

=> s l6 exa

```

SAMPLE SEARCH INITIATED 07:24:32 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

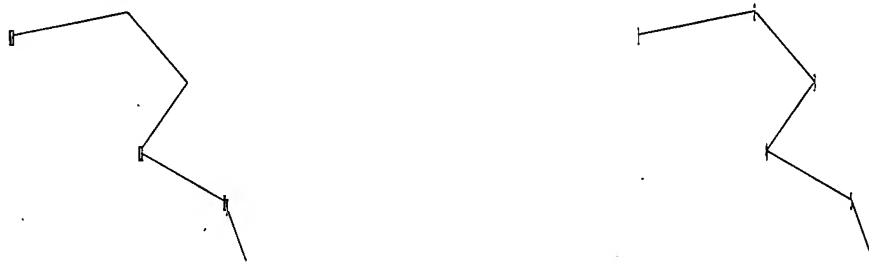
100.0% PROCESSED 5 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 5 TO 234  
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA EXA SAM L4

=>

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical  
Data\10814058\cmp 4.str



chain nodes :  
1 2 3 4 5 6  
chain bonds :  
1-2 2-3 3-4 4-5 5-6  
exact/norm bonds :  
1-2 3-4 4-5 5-6  
exact bonds :  
2-3

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:CLASS

L8 STRUCTURE UPLOADED

=> s 18

SAMPLE SEARCH INITIATED 07:27:23 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 149556 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2968301 TO 3013939  
PROJECTED ANSWERS: 112074 TO 121232

L9 50 SEA SSS SAM L8

=> s 18 exa

STRUCTURES CONTAINING VARIABLE NODES NOT VALID IN EXACT OR FAMILY SEARCH  
You have requested a full structure (EXA or FAM) search on a  
structure containing one of the special variable-atom symbols  
A, M, Q, or X, or a variable group G. Only bond variability

is allowed in structures for EXA or FAM searches. Variable nodes are never permitted.

=> s 19

SAMPLE SEARCH INITIATED 07:27:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 149556 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2968301 TO 3013939  
PROJECTED ANSWERS: 112074 TO 121232

L10 50 SEA SSS SAM L8

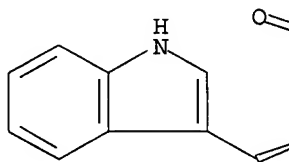
=> d 1-20

L10 ANSWER 1 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 920323-68-8 REGISTRY  
ED Entered STN: 09 Feb 2007  
CN L-Argininamide, L-norleucyl-L-cysteinyl-L-histidyl-D-phenylalanyl-L-  
arginyl-L-tryptophyl-4-aminobutanoyl-L-cysteinyl- $\beta$ -alanyl- $\beta$ -  
alanyl-L-tyrosylglycyl-L-arginyl-L-arginyl-L-arginyl-L-arginyl-L-  
glutaminyl-L-arginyl-L-arginyl-L-arginyl-, cyclic (2 $\rightarrow$ 8)-disulfide  
(CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C124 H205 N57 O24 S2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

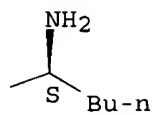
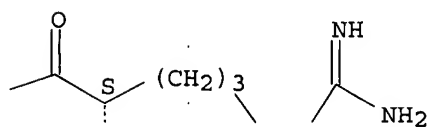
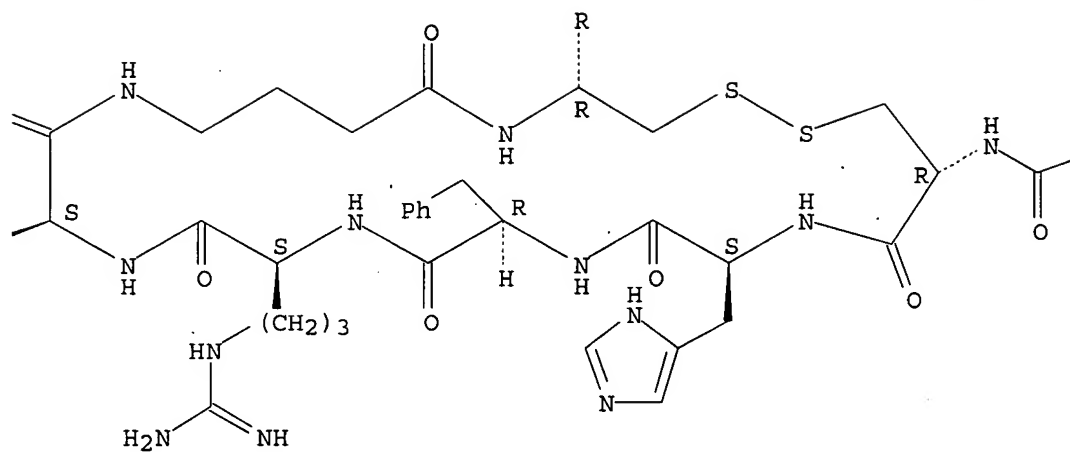
Absolute stereochemistry.

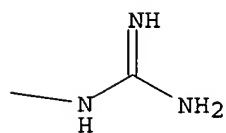
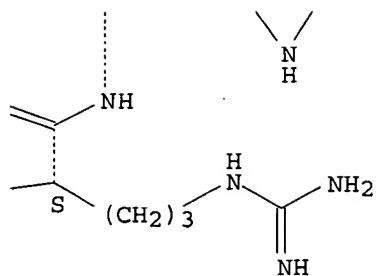
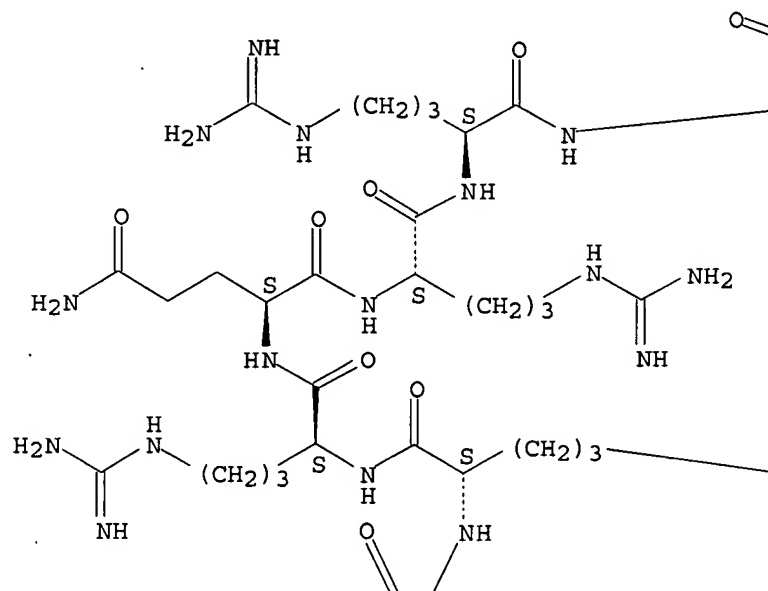
PAGE 1-A

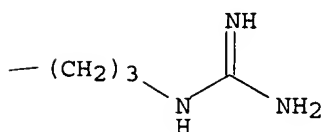
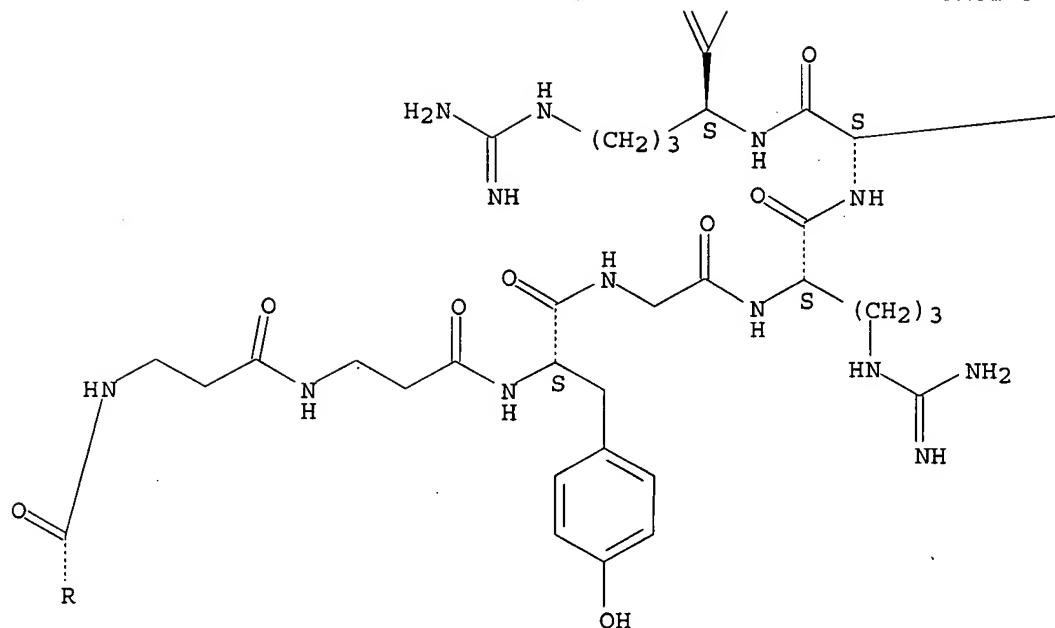


H<sub>2</sub>N



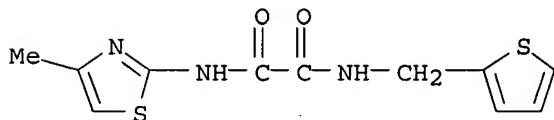






1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 920254-75-7 REGISTRY  
 ED Entered STN: 09 Feb 2007  
 CN Ethanediame, N1-(4-methyl-2-thiazolyl)-N2-(2-thienylmethyl)- (CA INDEX NAME)  
 MF C11 H11 N3 O2 S2  
 SR Chemical Library  
 Supplier: Aurora Fine Chemicals

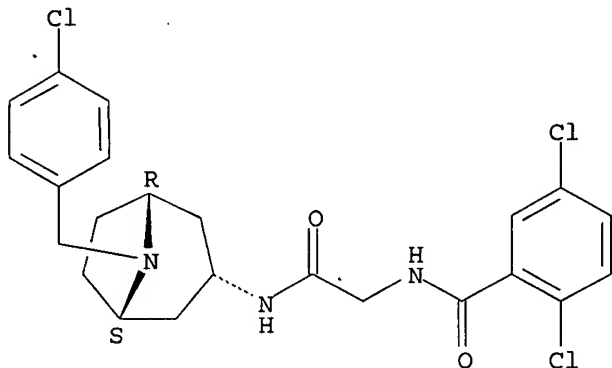


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 ANSWER 3 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 917106-88-8 REGISTRY  
 ED Entered STN: 10 Jan 2007  
 CN Benzamide, 2,5-dichloro-N-[2-[[[3-endo)-8-[(4-chlorophenyl)methyl]-8-

azabicyclo[3.2.1]oct-3-yl]amino]-2-oxoethyl]- (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C23 H24 Cl3 N3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS

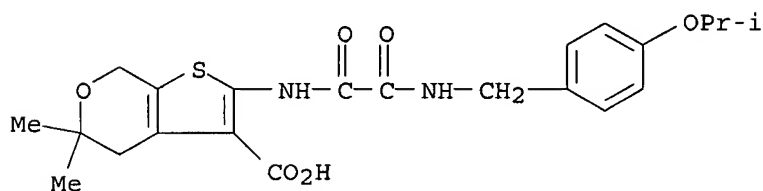
Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

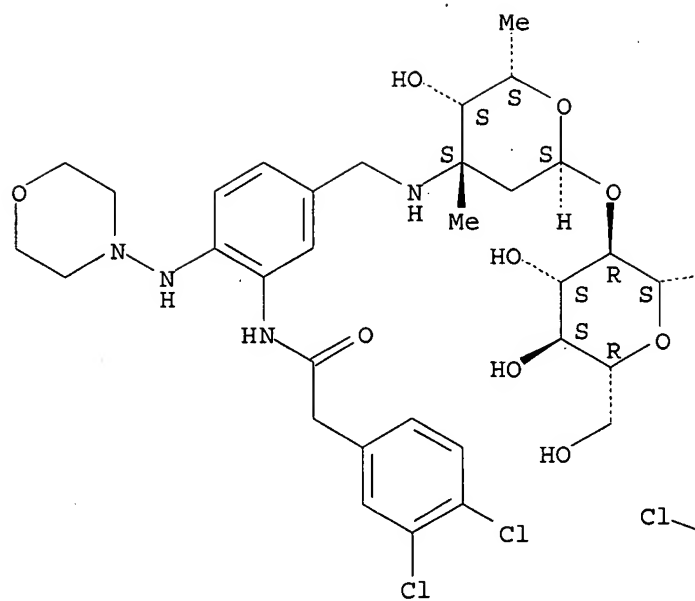
L10 ANSWER 4 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 903199-11-1 REGISTRY  
 ED Entered STN: 22 Aug 2006  
 CN 5H-Thieno[2,3-c]pyran-3-carboxylic acid, 4,7-dihydro-5,5-dimethyl-2-[[2-[[[4-(1-methylethoxy)phenyl]methyl]amino]-2-oxoacetyl]amino]- (CA INDEX NAME)  
 MF C22 H26 N2 O6 S  
 SR Chemical Library  
 Supplier: Interbioscreen Ltd.  
 LC STN Files: CHEMCATS

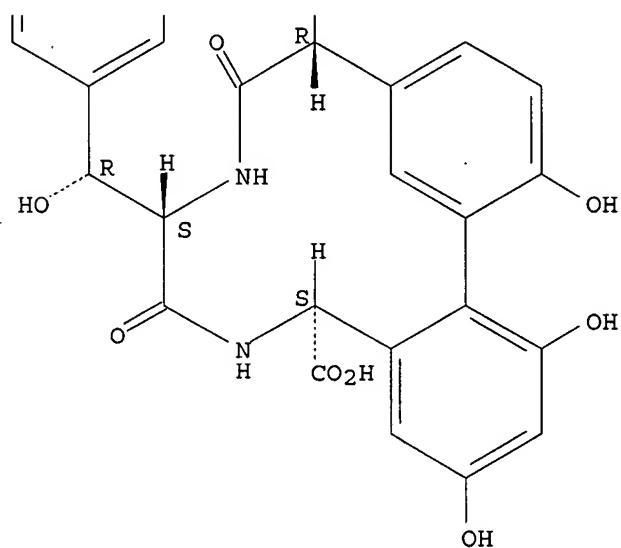
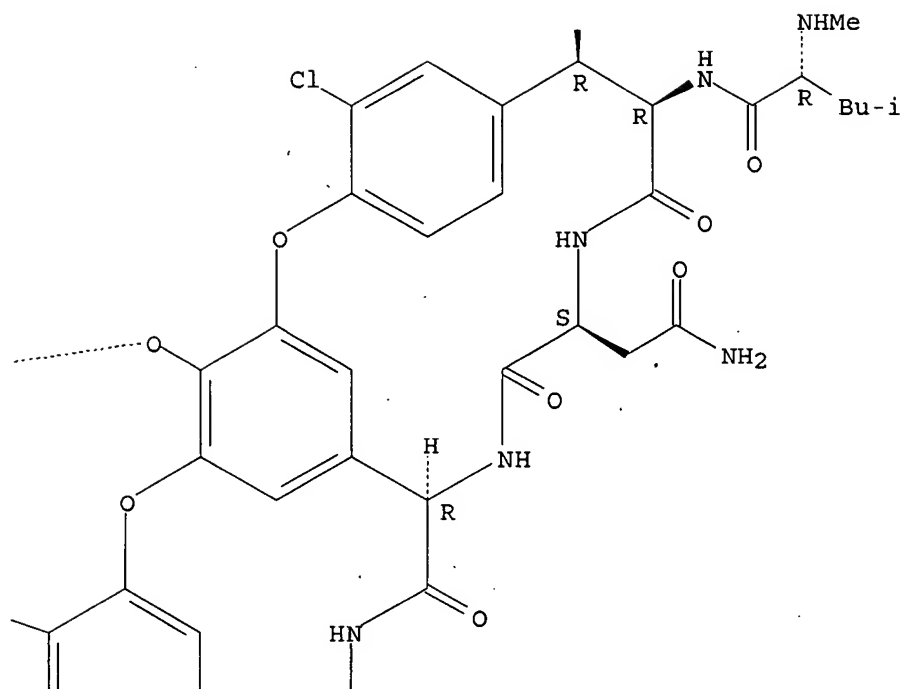


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 ANSWER 5 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 889936-52-1 REGISTRY  
 ED Entered STN: 29 Jun 2006  
 CN Vancomycin, N3'''-[[3-[[[(3,4-dichlorophenyl)acetyl]amino]-4-(4-morpholinylamino)phenyl]methyl]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C85 H94 Cl4 N12 O26  
 CI COM  
 SR CA

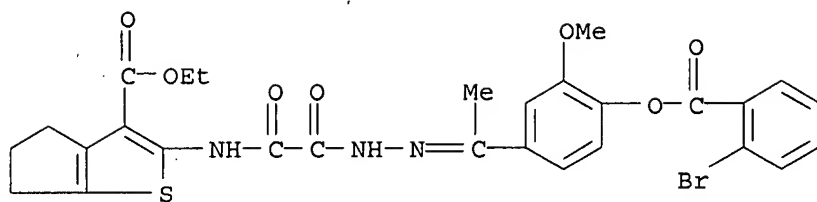
Absolute stereochemistry.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 ANSWER 6 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 885544-08-1 REGISTRY  
 ED Entered STN: 25 May 2006  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C28 H26 Br N3 O7 S  
 SR Chemical Library  
 Supplier: Scientific Exchange, Inc.  
 LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

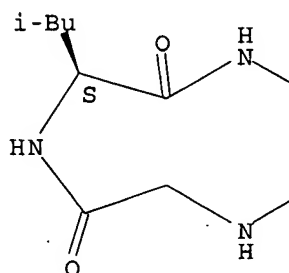
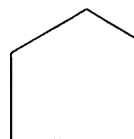
L10 ANSWER 7 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 880879-26-5 REGISTRY  
 ED Entered STN: 18 Apr 2006  
 CN L-Tyrosine, L-seryl-L- $\alpha$ -aspartyl-L-seryl-L-lysyl-L-isoleucylglycyl-L-asparaginylglycyl-L-cysteinyl-L-phenylalanylglycyl-L-phenylalanyl-L-prolyl-L-leucyl-L- $\alpha$ -aspartyl-L-arginyl-L-isoleucylglycyl-L-seryl-L-valyl-L-serylglycyl-L-leucylglycyl-L-cysteinyl-L-asparaginyl-L-seryl-L-phenylalanyl-L-arginyl-, cyclic (9 $\rightarrow$ 25)-disulfide (9CI) (CA INDEX NAME)

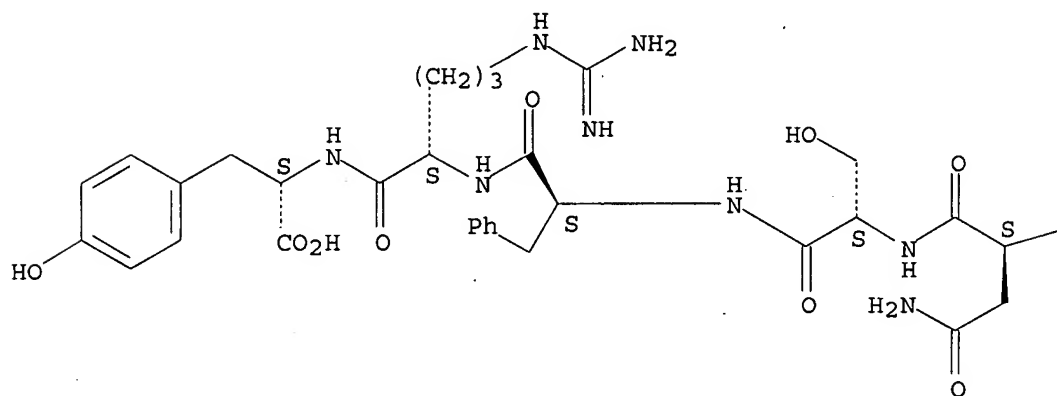
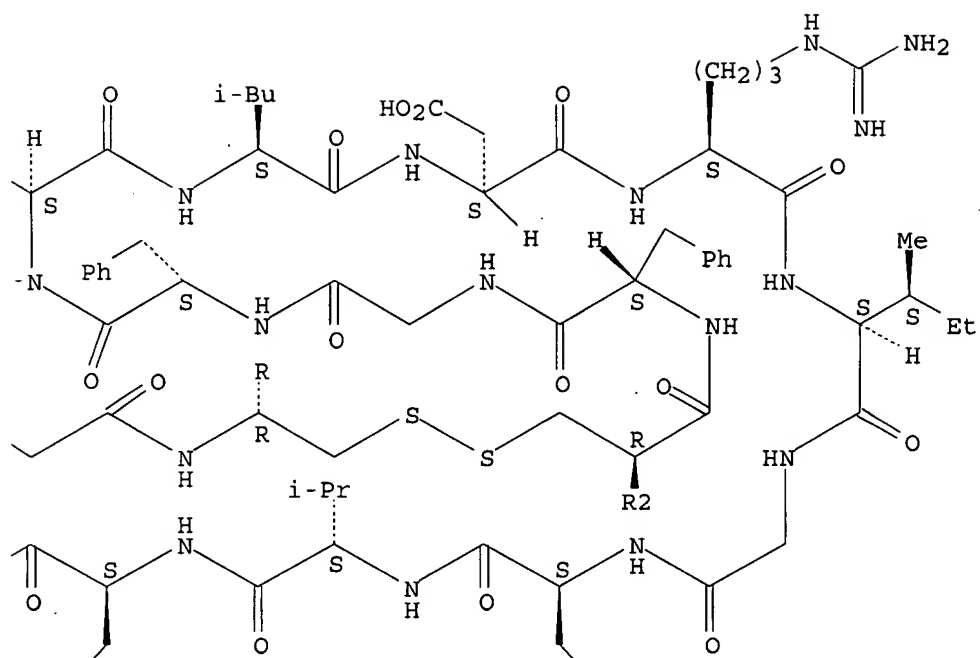
OTHER NAMES:

CN 112: PN: WO2006005140 SEQID: 126 claimed protein  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C137 H207 N39 O43 S2  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

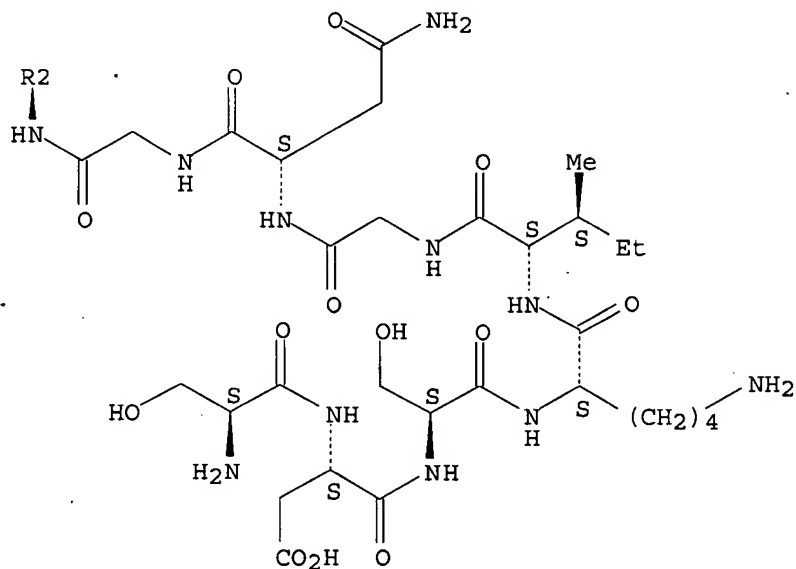
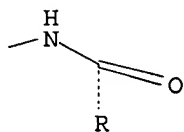
Absolute stereochemistry.

PAGE 1-B









1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

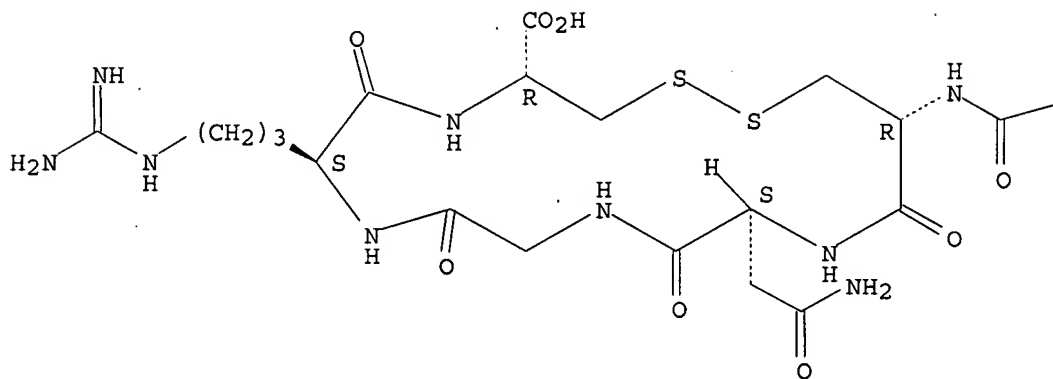
L10 ANSWER 8 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 872181-10-7 REGISTRY  
ED Entered STN: 19 Jan 2006  
CN L-Cysteine, N6-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]-L-lysylglycyl-L-cysteine-L-asparaginylglycyl-L-arginyl-, cyclic (3-7)-disulfide (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C47 H57 N13 O14 S3  
SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

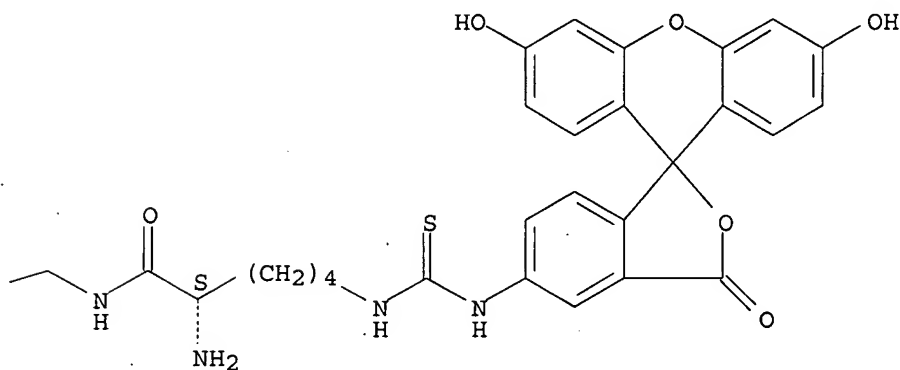
\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

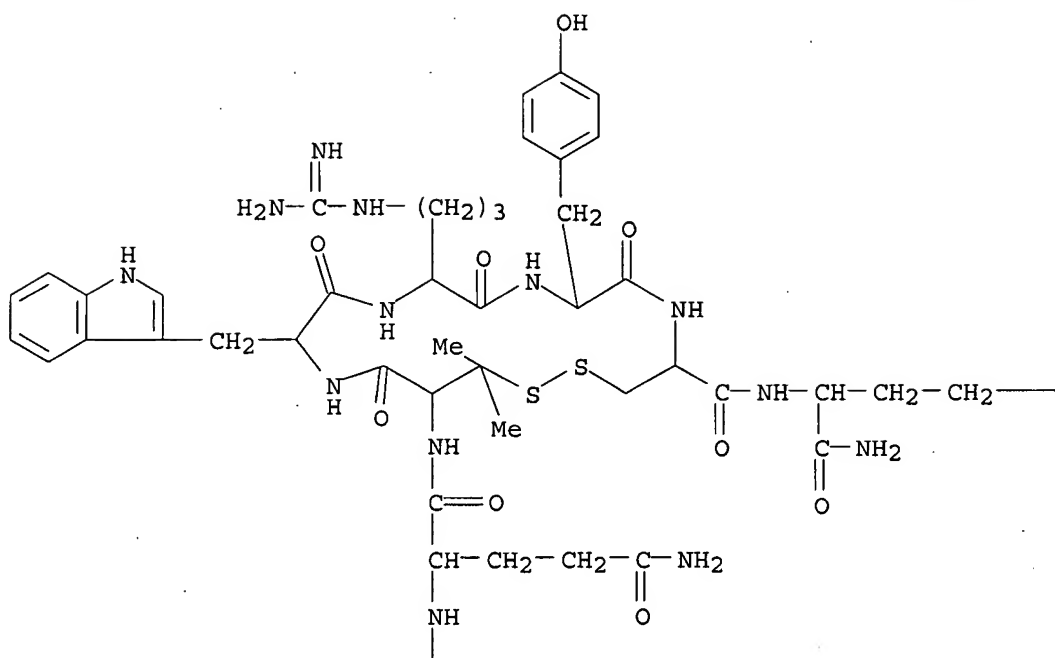


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

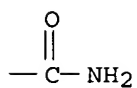
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 9 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 861888-37-1 REGISTRY  
ED Entered STN: 26 Aug 2005  
CN L-Glutamamide, N-acetyl-L-tyrosyl-L-glutaminyl-3-mercapto-L-valyl-L-tryptophyl-L-arginyl-L-tyrosyl-L-cysteinyl-, cyclic (3-7)-disulfide (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C55 H73 N15 O13 S2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

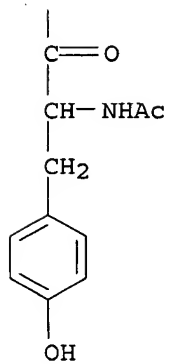
PAGE 1-A



PAGE 1-B



PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

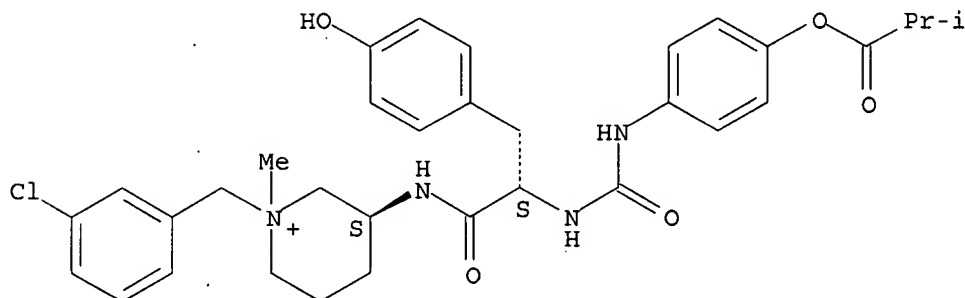
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
L10 ANSWER 10 OF 50  REGISTRY  COPYRIGHT 2007 ACS on STN
RN 854914-73-1  REGISTRY
ED Entered STN: 13 Jul 2005
CN Piperidinium, 1-[(3-chlorophenyl)methyl]-3-[[[(2S)-3-(4-hydroxyphenyl)-2-
[[[4-(2-methyl-1-oxopropoxy)phenyl]amino]carbonyl]amino]-1-
oxopropyl]amino]-1-methyl-, (3S)-, salt with trifluoroacetic acid (1:1)
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H40 Cl N4 O5 . C2 F3 O2
SR CA
LC STN Files: CA, CAPLUS
```

CM 1

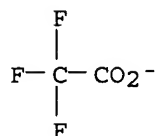
CRN 854914-72-0  
CMF C33 H40 Cl N4 O5

Absolute stereochemistry.



CM 2

CRN 14477-72-6  
CMF C2 F3 O2

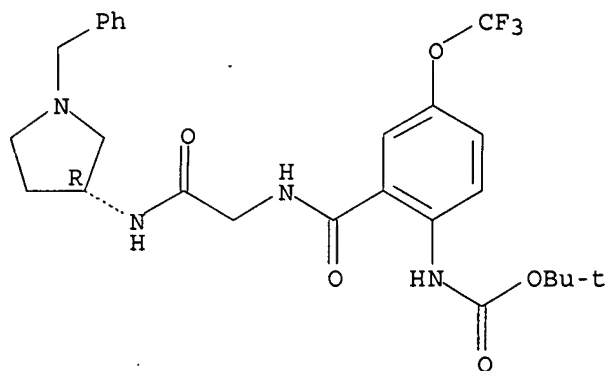


1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
L10 ANSWER 11 OF 50  REGISTRY  COPYRIGHT 2007 ACS on STN
RN 850412-33-8  REGISTRY
ED Entered STN: 13 May 2005
CN Carbamic acid, [2-[[[2-oxo-2-[[[(3R)-1-(phenylmethyl)-3-
pyrrolidinyl]amino]ethyl]amino]carbonyl]-4-(trifluoromethoxy)phenyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H31 F3 N4 O5
SR CA
```

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



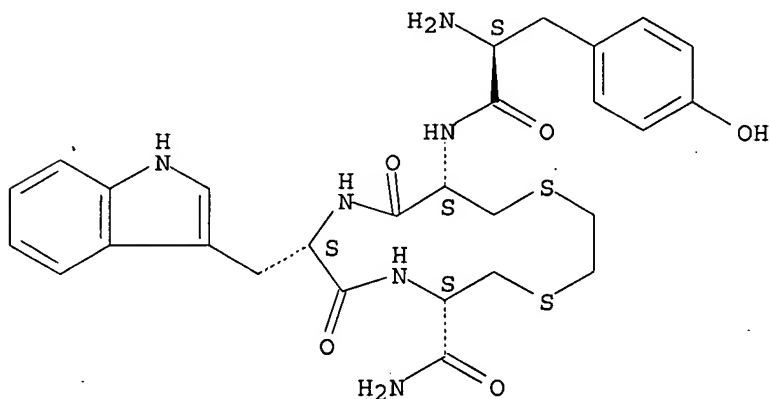
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 12 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 849242-48-4 REGISTRY  
ED Entered STN: 26 Apr 2005  
CN 1,4-Dithia-7,10-diazacyclotridecane-6-carboxamide, 12-[[[(2S)-2-amino-3-(4-hydroxyphenyl)-1-oxopropyl]amino]-9-(1H-indol-3-ylmethyl)-8,11-dioxo-, (6S,9S,12S)- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C28 H34 N6 O5 S2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

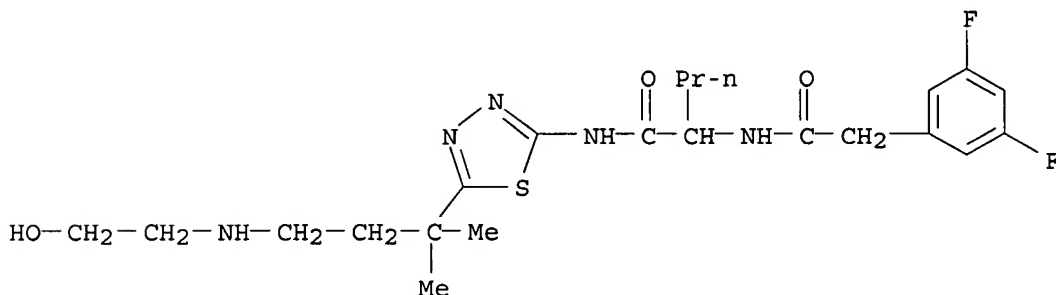


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 13 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 845898-97-7 REGISTRY  
ED Entered STN: 18 Mar 2005

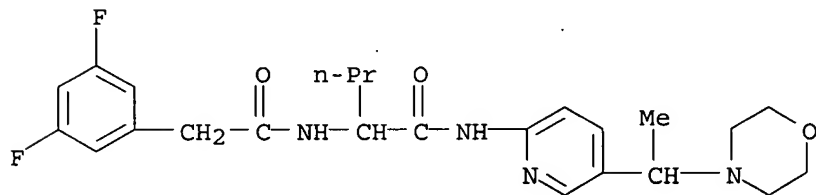
CN Benzeneacetamide, 3,5-difluoro-N-[1-[[[5-[3-[(2-hydroxyethyl)amino]-1,1-dimethylpropyl]-1,3,4-thiadiazol-2-yl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)  
 MF C22 H31 F2 N5 O3 S  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

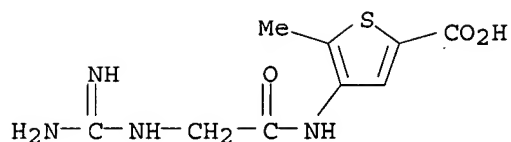
L10 ANSWER 14 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 843643-68-5 REGISTRY  
 ED Entered STN: 07 Mar 2005  
 CN Benzeneacetamide, 3,5-difluoro-N-[1-[[[5-[1-(4-morpholinyl)ethyl]-2-pyridinyl]amino]carbonyl]butyl]- (9CI) (CA INDEX NAME)  
 MF C24 H30 F2 N4 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

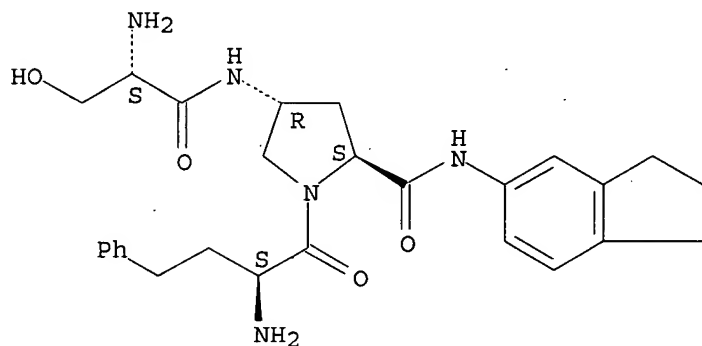
L10 ANSWER 15 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 802004-89-3 REGISTRY  
 ED Entered STN: 22 Dec 2004  
 CN 2-Thiophenecarboxylic acid, 4-(2-guanidinoacetamido)-5-methyl- (8CI) (CA INDEX NAME)  
 MF C9 H12 N4 O3 S  
 CI COM  
 SR CA



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

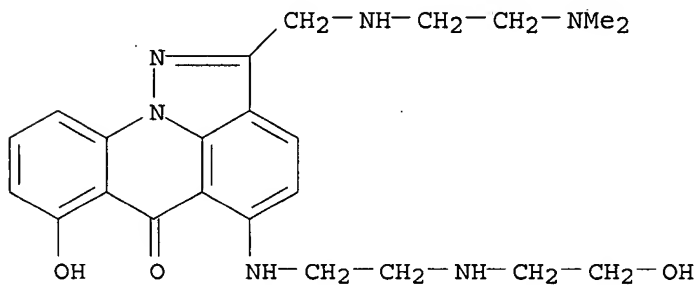
L10 ANSWER 16 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 785759-57-1 REGISTRY  
 ED Entered STN: 22 Nov 2004  
 CN 2-Pyrrolidinecarboxamide, 4-[[ (2S)-2-amino-3-hydroxy-1-oxopropyl]amino]-1-  
 [(2S)-2-amino-1-oxo-4-phenylbutyl]-N-(2,3-dihydro-1H-inden-5-yl)-,  
 (2S,4R)-(9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C27 H35 N5 O4  
 CI COM  
 SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

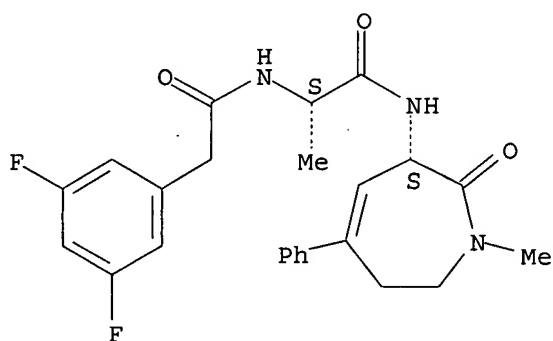
L10 ANSWER 17 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 770675-09-7 REGISTRY  
 ED Entered STN: 27 Oct 2004  
 CN 6H-Pyrazolo[4,5,1-de]acridin-6-one, 2-[[[2-(dimethylamino)ethyl]amino]meth  
 yl]-7-hydroxy-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]- (9CI) (CA INDEX  
 NAME)  
 MF C23 H30 N6 O3  
 CI COM  
 SR CA



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 ANSWER 18 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 762291-00-9 REGISTRY  
ED Entered STN: 14 Oct 2004  
CN Benzeneacetamide, 3,5-difluoro-N-[(1S)-1-methyl-2-oxo-2-[[[(3S)-2,3,6,7-tetrahydro-1-methyl-2-oxo-5-phenyl-1H-azepin-3-yl]amino]ethyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H25 F2 N3 O3  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



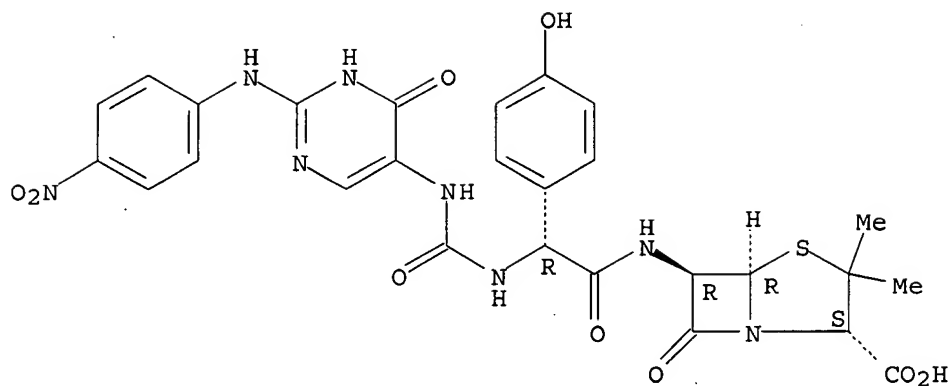
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 19 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
RN 757138-32-2 REGISTRY  
ED Entered STN: 05 Oct 2004  
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[1,4-dihydro-2-[(4-nitrophenyl)amino]-4-oxo-5-pyrimidinyl]amino]carbonyl]amino](4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2 $\alpha$ ,5 $\alpha$ ,6 $\beta$ (S\*)]]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C27 H26 N8 O9 S  
CI COM  
SR CA

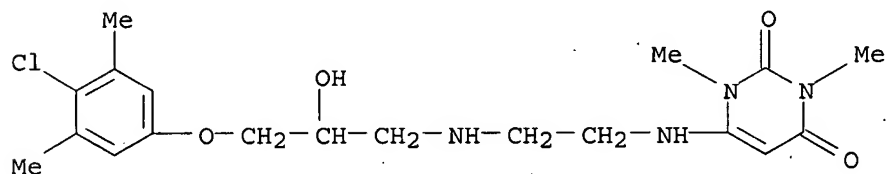
Absolute stereochemistry.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L10 ANSWER 20 OF 50 REGISTRY COPYRIGHT 2007 ACS on STN  
 RN 748734-75-0 REGISTRY  
 ED Entered STN: 20 Sep 2004  
 CN 2,4(1H,3H)-Pyrimidinedione, 6-[[2-[[3-(4-chloro-3,5-dimethylphenoxy)-2-hydroxypropyl]amino]ethyl]amino]-1,3-dimethyl- (9CI) (CA INDEX NAME)  
 MF C19 H27 Cl N4 O4  
 CI COM  
 SR CA



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

303.35

303.77

STN INTERNATIONAL LOGOFF AT 07:43:04 ON 07 MAY 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptamxg1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals  
NEWS 3 JAN 16 CA/CAPLUS Company Name Thesaurus enhanced and reloaded  
NEWS 4 JAN 16 IPC version 2007.01 thesaurus available on STN  
NEWS 5 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data  
NEWS 6 JAN 22 CA/CAPLUS updated with revised CAS roles  
NEWS 7 JAN 22 CA/CAPLUS enhanced with patent applications from India  
NEWS 8 JAN 29 PHAR reloaded with new search and display fields  
NEWS 9 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases  
NEWS 10 FEB 15 PATDPASPC enhanced with Drug Approval numbers  
NEWS 11 FEB 15 RUSSIAPAT enhanced with pre-1994 records  
NEWS 12 FEB 23 KOREAPAT enhanced with IPC 8 features and functionality  
NEWS 13 FEB 26 MEDLINE reloaded with enhancements  
NEWS 14 FEB 26 EMBASE enhanced with Clinical Trial Number field  
NEWS 15 FEB 26 TOXCENTER enhanced with reloaded MEDLINE  
NEWS 16 FEB 26 IFICDB/IFIPAT/IFIUDB reloaded with enhancements  
NEWS 17 FEB 26 CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases  
NEWS 18 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 19 MAR 16 CASREACT coverage extended  
NEWS 20 MAR 20 MARPAT now updated daily  
NEWS 21 MAR 22 LWPI reloaded  
NEWS 22 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 23 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 24 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 25 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 26 APR 30 CA/CAPLUS enhanced with 1870-1889 U.S. patent records  
NEWS 27 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 28 MAY 01 New CAS web site launched

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:42:21 ON 07 MAY 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.63

0.63

FILE 'REGISTRY' ENTERED AT 09:43:52 ON 07 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

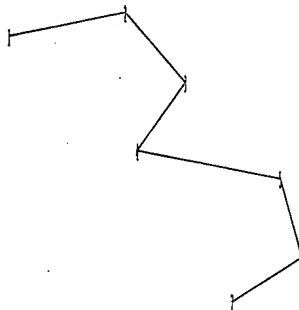
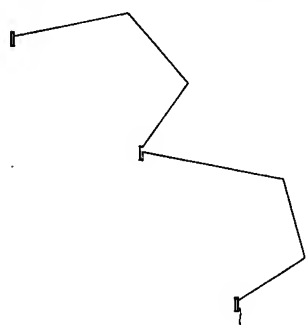
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\mgraffeo\My Documents\Critical Data\10814058\cmp 5.str



chain nodes :

1 2 3 4 5 6 7

chain bonds :

1-2 2-3 3-4 4-5 5-6 6-7

exact/norm bonds :

1-2 3-4 4-5 6-7

exact bonds :  
2-3 5-6

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS

L1 STRUCTURE UPLOADED

=> file reg	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.45	1.08

FILE 'REGISTRY' ENTERED AT 09:44:04 ON 07 MAY 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6  
DICTIONARY FILE UPDATES: 6 MAY 2007 HIGHEST RN 934336-20-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> s l1  
SAMPLE SEARCH INITIATED 09:44:07 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 94634 TO ITERATE

2.1% PROCESSED 2000 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 1874416 TO 1910944  
PROJECTED ANSWERS: 746386 TO 769650

L2 50 SEA SSS SAM L1

=> s l1 exa  
SAMPLE SEARCH INITIATED 09:44:15 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH      \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:      44 TO      476  
PROJECTED ANSWERS:      1 TO      80

L3                    1 SEA EXA SAM L1

=> d

L3    ANSWER 1 OF 1    REGISTRY    COPYRIGHT 2007 ACS on STN  
RN    756798-35-3    REGISTRY  
ED    Entered STN:    05 Oct 2004  
CN    1,2-Ethanedi(amine-15N), N-[2-(amino-15N)ethyl]- (9CI)    (CA INDEX NAME)  
MF    C4 H13 N3  
CI    COM  
SR    CA

$^{15}\text{NH}_2\text{---CH}_2\text{---CH}_2\text{---}^{15}\text{NH---CH}_2\text{---CH}_2\text{---}^{15}\text{NH}_2$

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.40	3.48

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:44:40 ON 07 MAY 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 7 May 2007    VOL 146 ISS 20  
FILE LAST UPDATED: 6 May 2007    (20070506/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l3

L4                    0 L3

=> s 756798-35-3/rn

0 756798-35-3

0 756798-35-3D

L5                    0 756798-35-3/RN

(756798-35-3 (NOTL) 756798-35-3D )

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.49

7.97

STN INTERNATIONAL LOGOFF AT 09:45:33 ON 07 MAY 2007